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A MODEL OF ORGANIC CHEMICAL FATE IN A BIOLOGICAL WASTEWATER TREATMENT PLANT

R.A.C. PROJECT NO.149 PL

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ABSTRACT

A model, based on the fugacity concept, has been developed to correlate and predict the steady state phase concentrations, process stream fluxes and fate of organic chemicals in a biological wastewater treatment plant. Input data consist of the relevant physical properties of the chemicals and the plant's design and operating parameters. It is algebraically simple, robust and can be run on a personal computer.

The model estimates the relative amounts of chemical which are stripped or volatilized, sorbed to sludge, biodegraded, and discharged in the effluent water. Calibration and validation of the model has been attempted by comparing the model output with data from a laboratory scale treatment system, with output from other similar models, and with data from full scale plants. The most critical variable is the biodegradation rate constant and its dependence on biomass concentration.

It is believed that with further calibration and validation, the model will be a useful tool for assessment of chemical fate in sewage treatment systems.

Copies of the program on diskette are available from the authors and from the Ministry of the Environment.

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INTRODUCTION

Some fifty thousand organic chemicals have been produced commercially, and approximately 1200 new chemicals are introduced each year (1). Many of these are of concern because of their toxicity and their tendency to accumulate in biota, and hence reach concentrations which are toxic or which render biota inedible (2,3). A substantial fraction of the organic chemicals used in industry, commerce, and domestically are discharged to sewer systems, where they are subsequently treated in sewage treatment plants (STPs). This issue has been comprehensively reviewed recently by Grady (4) who has assessed the state of the art, discussed research priorities, and provided an extensive bibliography. Monteith (5) has reviewed the frequency of occurrence removal and variability in concentration of these contaminants.

It is important to establish within regulatory agencies the capability of assessing, for existing and new chemicals, the fractions of the chemical present in the plant influent which are ultimately degraded, air-stripped, sorbed to sludge (which may be disposed of by land spreading or incineration), and which leave in the effluent water. Mere removal from the water may not represent a complete solution to the problem of environmental contamination - it may represent only a relocation of the problem. If the effluent is judged to have an intolerable concentration of a specific chemical, it may be possible to change plant operating conditions to improve performance, or it may be necessary to restrict sewer discharges. A mass balance model describing the chemical's fate in a STP is thus an

invaluable component of such control measures. This predictive capability has been discussed by Blackburn (6) and others.

Under optimal operating conditions, a biological treatment plant may remove a large percentage, eg. 70 to 100%, of organic pollutants from the sewage, thus reducing the burden of these contaminants on the environment (4). It is also known that treatment efficiency is variable and that certain operating parameters, such as sludge retention time (SRT), influence the removal efficiency (7). To improve the performance of STPs, the reasons that such factors influence the fate of organic chemicals during treatment must be known.

In this study, we describe and discuss development of a steady-state model which seeks to correlate or predict the fate, and thus the important removal mechanisms, of organic chemicals in a STP. The model is based on the fugacity modeling concept, which has been successfully used to describe the fate of organic chemicals in the environment (8). The model has been designed to be easy to understand and use; it is programmed in BASIC language, and is compatible with an IBM Personal Computer. The input parameters are the physical properties of the chemical (molecular weight, vapor pressure, solubility in water, octanol-water partition coefficient, and biodegradation rate constant) and the relevant design and operating parameters of the biological wastewater treatment plant (water flow rates, solids content in process streams and in reactors, volatile matter content of solids, and geometry of the vessels). The program gives as output a prediction of the chemical fluxes in all process streams, the chemical concentration in the water, air, and sludge phases, and a statement of mass balance.

The model contains features which have been included in other similar models, notably those of Blackburn et al. (9), Roberts et al. (10), and Kincannon and Stover (11, 12). It is not claimed to provide an accurate description of chemical fate, nor does it in its present form describe transient behaviour, but it is believed to be based on sound physical chemical principles and thus, with suitable parameterization, should describe the system in a reasonable, robust fashion. We expect, and hope, that it will be modified and improved as more treatment data become available. It is thus regarded as one step, along one possible route towards a comprehensive, validated capability of modelling organic chemical fate in STPs.

A key issue in any model development is that of validation, i.e. an assessment of the fidelity with which the model can describe real systems, and preferably systems which were not used in its calibration or parameterization. In this study several validation efforts were attempted.

First a model activated sludge system was designed, built and operated in the laboratory and the fates of selected organic chemicals (toluene, pyrene, phenol, dichlorobenzene, naphthalene, pentachlorophenol and lindane) were studied. The results of these studies have been reported by Clark (13), who also tested the model against these results. It was concluded that the model could describe the observed phenomena, but that the system was a severe over-simplification of a real STP, thus the validity of the model when applied to real systems could not be judged.

Second, Clark compared the models such as those of Blackburn (6, 9) and Roberts et al. (10) and found general correspondence. This is not surprising in view of the similar nature of the equations. Again this does not demonstrate that the model is predictive of real systems.

Third, the model was used to compare the computed fate with that of selected chemicals in real STPs as reviewed by Monteith (5). The results of this comparison are included in this report. It must be appreciated that it is unlikely that any simple mathematical model will ever accurately predict the fate of organic chemicals in STPs. Flows and concentrations vary continuously as do temperatures and the nature of the microbial community which is primarily responsible for sorption and degradation. The best that can be hoped for is that the model gives a reasonable representation of long term or average fate, and enables the dominant processes and fate mechanisms to be identified.

REMOVAL MECHANISMS OF ORGANIC CHEMICALS

In a conventional biological treatment plant, illustrated in Figure 1, the raw sewage is purified in two major steps: primary sedimentation and secondary or biological treatment.

During primary sedimentation, the settleable suspended solids are removed in a regime of low horizontal velocities by gravity settling with a 60 to 75% efficiency. Solids which accumulate at the bottom of the tank are removed periodically, usually once every 2 to 8 hours. During this time, the solids concentration of the sludge increases to 3-5%, which allows for the wasting of a small volume of sludge, representing possibly 60 to 75% of the incoming suspended solids (14). The primary purpose of suspended solids removal is to reduce the organic load on the biological system since these solids contain 60-70% volatile or organic matter which is substantially biodegradable.

Organic chemicals present in the influent thus experience the fate of being (i) removed with the deposited sludge, or (ii) dissolved or sorbed to solids in the water phase which flows to subsequent treatment, or (iii) volatilized through the water surface into the air, or (iv) biodegraded. Biodegradation usually plays a minor role in primary tanks, unless the organic chemical is very susceptible to anaerobic degradation.

During the biological treatment step, biodegradable organic matter is incorporated into the biomass and metabolized by aerobic and facultative anaerobic bacteria. Biological activity

in the aeration tank requires oxygen which is supplied either from air diffused through the aeration tanks or from surface aerators. This diffused air also keeps the tank contents well mixed. Usually, the aeration rate is controlled by the oxygen demand of the purification process. The organic chemicals may be biodegraded as a result of contact with activated sludge, which is kept in the system for a retention time which may range from 2 to 6 days for conventional activated sludge systems, and ideally has enough time to become acclimated to the chemical (7, 14, 15). Undegraded chemical partitions between water, the biomass and air, thus leaving the system in the effluent or by volatilization.

In the final settling tank, the biomass is separated from the purified water by gravity settling under steady, low flow velocity conditions. Most of the settled sludge is returned to the aeration tank (70-100% of plant inflow) to maintain an activated sludge concentration of 2000 to 4000 g/m^3 (14). The return sludge also carries some of the sorbed organic chemicals back into the aeration tank. The suspended solids content of 8000 to 10,000 g/m^3 of settled biological sludge depends on several operating parameters, such as food to microorganism ratio (F/M ratio), Mixed Liquor Suspended Solids content (MLSS) in the aeration tank, recycle ratio and mixed liquor flow rate.

Sludge is typically retained in the final settling tank for 1 to 4 hours, a short enough time that a sufficient amount of oxygen remains in the sludge to sustain the metabolic activity of the biomass. A small fraction of settled sludge is wasted from the system at this location. In the final settling tank, organic chemicals are volatilized, biodegraded, are discharged in the plant effluent and waste or are recycled in the return sludge.

Model Structure

The objective of the model is to quantify the fate or mass balance of a specified chemical in this system as illustrated in Figure 1. The model is a set of steady state, mass balance equations describing the flows and amounts of water, biological solids, air and chemical throughout the system. Sufficient data are provided on flowrates, volumes and concentrations to define the water, air and solids mass balances.

All parameters and symbols are designated to facilitate identification and interpretation. Flow rates have an initial G followed by W for water, A for air or S for solids, then followed by a number defining the stream. GW9 is thus the flowrate (m^3/h) of water in stream 9. A final G designates that the solid flow is in units of g/h. Values typical of a 1000 m^3/h STP have been included in the model, but they can be varied if desired to meet specific requirements. Chemical flows are designated M mol/h or MG g/h followed by the stream number. Solid concentrations are designated S g/m^3 and chemical concentrations as CG g/m^3.

The program is structured to be user-interactive. The user first inputs the physical chemical properties of the substance of interest in one of three ways. The chemical properties may be user-specified, a previously specified chemical may be tested again, or a set of properties may be drawn from a file containing data for eighteen commonly encountered chemicals.

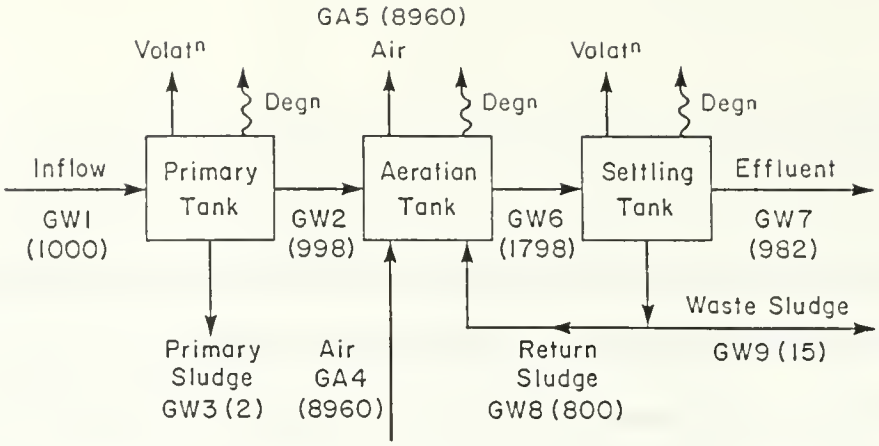

FIGURE IA WATER BALANCE (m^3/h)

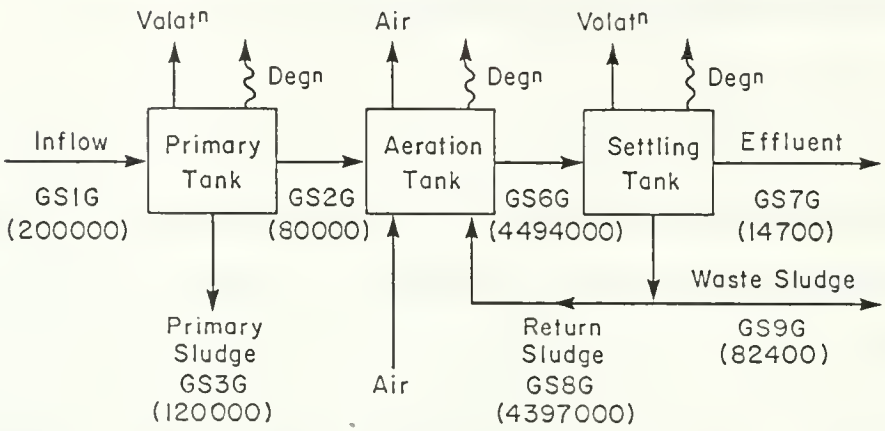

FIGURE IB SOLIDS BALANCE (g/h)

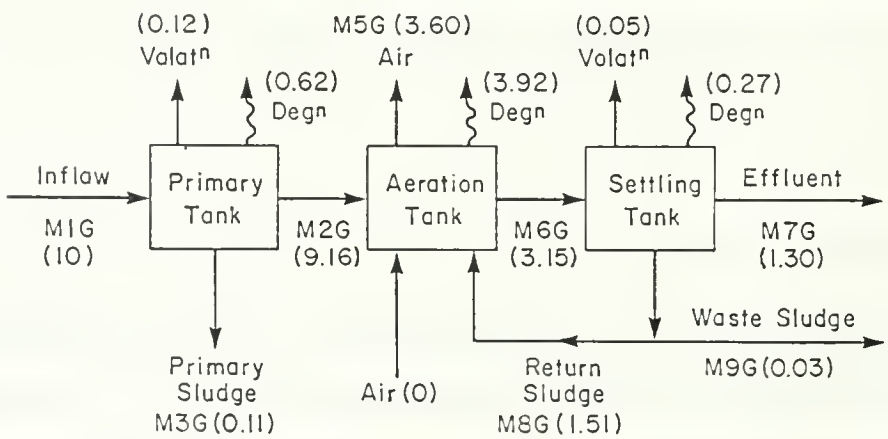

FIGURE IC CHEMICAL BALANCE (g/h)

Figure 1 Diagram of STP with water, solids and chemical balances corresponding to the output for toluene in Figure 4.

Second, the user specifies the STP operating conditions with similar options, i.e. user-specified, previously specified or default conditions representing a typical STP.

Finally, the STP design dimensions of vessel areas, depth and volumes are specified with the same three options applicable to the operating conditions.

An option is included to select the nature and extent of the printed output.

After the output is printed the program returns to the start and requests new input. Obviously "previously specified" values can not be used in the first run.

This approach enables the user to test various chemicals on the same STP or vary STP conditions for a given chemical.

Figures 2 and 3 illustrate the screen commands used to input data to the program. The STP operating conditions are determined as follows.

The area and depth (and hence volume) of the primary clarifier and final clarifier or settling tank are specified. Default values are used assuming depths of both vessels of 3.8 m (12.5 ft) and overflow rates of 90 (primary) and 33 (final) m^3/m^2 day based in the inflow. The aeration tank volume is specified, or set to give an 8 hour retention to the inflow. These are typical design or operating values recommended by the Ontario Ministry of the Environment (15).

```
        PREDICTED FATE OF AN ORGANIC CHEMICAL IN A
        WASTEWATER TREATMENT FACILITY


Input Chemical Properties
Specify a chemical by entering one of the following
A chemical to be user-specified  1
A chemical previously specified  2
A chemical from the following list
Benzene(3), toluene(4), 1,1,2  trichloroethene(5), 1,1,1 trichloroethane(6)
1,4 dichlorobenzene(7), naphthalene(8), pyrene(9), phenol(10),
2-4D (11), gamma BHC (12) ,butyl-benzyl phthalate (13)
di-butyl phthalate (14),di-octyl phthalate (15),2 ethyl hexyl phthalate (16),
pentachlorophenol (17),anthracene (18)
? 1

INPUT CHEMICAL PROPERTIES, ANY PREVIOUS VALUES IN PARENTHESES ( )
CHEMICAL NAME (preferably in CAPITALS)()
? TEST-CHEMICAL
TEMPERATURE deg C ( 0 )
? 20
MOLECULAR WEIGHT g/mol ( 0 )
?

200
WATER SOLUBILITY g/m3 ( 0 )
? 33
VAPOR PRESSURE Pa ( 0 )
? 3.5
LOG OCTANOL-WATER PARTITION COEFFICIENT KOW ( 0 )
? 4.2
BIODEGRADATION DATA IS REQUESTED NEXT. FOR YOUR GUIDANCE THE FOLLOWING
HALF LIVES MAY BE SELECTED AS INDICATIVE OF BIODEGRADABILITY
  RAPIDLY DEGRADABLE  1 HOUR
  MODERATELY DEGRADABLE  3 HOURS
  SLOWLY ,BUT SIGNIFICANTLY,DEGRADABLE  10 HOURS
  VERY SLOWLY DEGRADABLE  30 HOURS
BIODEGRADATION HALF LIFE AT MLSS OF 2000 mg/L (h) AT CONDITIONS IN
  PRIMARY CLARIFIER ( 0 )
? 24
  AERATION VESSEL   ( 0 )
? 8
  FINAL SETTLING TANK ( 0 )
? 8
```

Figure 2 Screen commands for entering chemical properties.

```
Specify STP operating conditions by entering one of the following
Conditions to be user-specified      1
Conditions previously specified      2
Default conditions                   3

? 1
INFLUENT RATE m3/h ( 0 )
? 1500
INFLUENT VSS g/m3 ( 0 )
? 30
FRACTIONAL REMOVAL OF VSS IN PRIMARY SLUDGE ( 0 )
? .75
VSS CONCENTRATION IN PRIMARY SLUDGE g/m3 ( 0 )
? 8000
SLUDGE RECYCLE AS FRACTION OF INFLUENT ( 0 )
? 2
WASTE SLUDGE AS FRACTION OF INFLUENT ( 0 )
? .015
MLSS CONCENTRATION IN AERATION VESSEL g/m3 ( 0 )
? 2500
VSS CONCENTRATION IN EFFLUENT g/m3 ( 0 )
? 5
AIR FLOW AS MULTIPLE OF AERATION TANK VOL/HOUR ( 0 )
? 1.2
CHEMICAL CONCENTRATION IN INFLUENT g/m3 ( 0 )
? 0.01

Specify STP design by entering one of the following
Design to be user-specified      1
Design previously specified      2
Default design                   3

? 1
INPUT STP DESIGN VALUES, ANY PREVIOUS VALUES IN PARENTHESES ( )
PRIMARY CLARIFIER AREA m2 ( 0 )
? 300
PRIMARY CLARIFIER DEPTH m ( 0 )
? 4
AERATION TANK VOLUME  m3 ( 0 )
? 9000
FINAL CLARIFIER AREA m2 ( 0 )
? 800
FINAL CLARIFIER DEPTH m ( 0 )
? 3
Specify desired printed output by entering 0 (zero) for NO and 1 (one) for YES
PART 1: CHEMICAL PROPERTIES,Z & D VALUES
? 1
PART 2: SPECIFICATIONS OF VESSELS,CONTENTS & STREAMS
? 1
PART 3: OVERALL MASS BALANCE
? 1
PART 4: FLOWSHEET
? 1
PART 5: NARRATIVE SUMMARY
? 1
```

Figure 3 Screen commands for entering STP operating conditions and design, and specifying output.

The water balance for the entire system is established as shown in Figure 1A by defining (or using default values given in parentheses) the flow rates for the inflow GW1 (as 1000 m^3/h), GW8 (return sludge) as a specified fraction (80%) of GW1, GW9 (waste activated sludge) as a specified fraction (1.5%) of GW1, and GW3 (primary sludge) as the volume necessary to waste a specified fraction (60%) of the incoming solids at a specified concentration of (50,000 g/m^3 or 5%). The other water flows are deduced by difference.

The air flows GA4 and GA5, also shown in Figure 1A, are set at a multiple (1.12) of the volume of the aeration tank per hour, i.e. 8960 m^3/h. This corresponds to 0.33 m^3 per 1000 m^3 of tank volume per second which is again a typical design value (16).

The solids balance, shown in Figure 1B, is established by specifying the influent solids concentration (200 g/m^3), i.e. the default influx of solids is 200 kg/h. Of this, a specified fraction (60% or 120 kg/h) leaves in the primary sludge as GS3 and the remainder passes to the aeration tank as GS2. A precise solids balance is not possible in subsequent stages because of biological growth and decay, thus the following approach is used. The mixed liquor suspended solids concentration in the aeration tank and its effluent have a specified default value (2500 g/m^3) which defines GS6. The effluent solids content is specified (15 g/m^3) to define GS7. The difference is split between streams 8 and 9 in the proportions of the water flows. Non-volatile or non biological solids are assumed to leave in the primary sludge and play no role in determining the dynamics of the organic chemical.

Another configuration could be accommodated in which all the waste sludge (Stream 9) is recycled to the primary tank. This involves changes to the equations which can be readily deduced.

The essential task of the model is to first establish these water air and biomass balances, then deduce from them the mass balance or fate of the chemical of interest (Figure 1C), solely from a knowledge of the influent concentration and the following physical chemical properties:

Molecular mass

Water solubility

Vapor pressure

Octanol-water partition coefficient

Biodegradation rate constant of chemical present in the biomass in each vessel

The following assumptions are made.

Equilibrium partitioning (equal fugacity) is assumed to exist for the chemical between the water and biomass phase in each tank. This assumption is believed to be reasonable, since for most organic chemicals, equilibrium is substantially approached during the treatment residence time of one or more hours. In the aeration tank, the off-gas stream is assumed to reach equilibrium with the water phase. This equilibrium assumption is widely used in predictive models for organic chemical fate in STPs (9).

The chemical entering the treatment plant and flowing to subsequent stages is either dissolved in the water, or sorbed on to the associated suspended solids. Once the wastewater enters the settling tank, the prevailing conditions determine the distribution of chemical between these phases.

Equations used in the model to describe chemical partitioning between phases are similar to or based on those proposed by Blackburn (6, 9), and Roberts (9) for sorption, volatilization and stripping.

The aeration tank is assumed to operate as a single completely stirred reactor. Plug flow aeration systems are believed to be more efficient in the stabilization of soluble organic wastes than stirred tank systems, thus the model gives a conservative estimate of performance. In practice, true plug flow conditions are difficult to achieve because of longitudinal dispersion, which tends to reduce differences in treatment efficiency in the two models. It would be relatively easy to modify the model to incorporate a sufficient number of multiple stirred tanks to reproduce near-plug flow behaviour.

The principal uncertainty is the calculation of biodegradation rate. The first order or linear version of the Monod equation is used which is believed to apply at low chemical concentrations. More complex equations could be substituted if data are available to justify their use.

The input data requested are the half lives of the chemical (h) under conditions when biomass is present at a MLSS concentration of 2000 g/m^3 in each vessel. Generally similar values are expected for the aerated conditions existing in the aeration tank and final clarifier, but a longer half life (slower rate) may apply to the primary clarifier in which anaerobic conditions may prevail. The program calculates first order rate constants for degradation in the biomass phase by assuming that equilibrium biomass-water partitioning applies at the MLSS of 2000 g/m^3. It then applies these rate constants to the volumes of biomass in each vessel. This automatically adjusts the rate (linearly) in proportion to MLSS concentration.

It is assumed that the biomass is fully acclimated to the chemical which is believed to be valid for sludge retention times of the order of several days.

The model solves the linear mass balance equations written around each tank, which include expressions for partitioning of the chemical between air, water, and biomass, and biodegradation in the biomass phases. The output consists of concentrations, flowrates and statement of the relative importance of the removal mechanisms; volatilization, stripping, biodegradation, sludge wasting and outflow in the effluent. These equations can be written in concentration form or in fugacity form, both being ultimately algebraically identical. However, the final conventional equations are lengthy and difficult to follow. On the other hand, the fugacity format equations are more compact and elegant, and the mass balance can easily be understood. It is appropriate here to digress to describe the fugacity approach in more detail.

The Fugacity Approach

Fugacity can be regarded as the escaping tendency (with units of pressure Pa) of an organic chemical from a phase, such as water, air, and biomass. In the air phase, it is equal to partial pressure. If a system is in equilibrium, ie. there is no net diffusion of chemical from one phase to the other, the fugacities of the chemical in each phase are equal, just as chemical potentials are equal. In effect, fugacity is a criterion of equilibrium related to chemical potential but it is more convenient in that it is linearly or near-linearly related to concentration (8).

In the model, fugacity (f Pa) is used as a surrogate for concentration, C (mol/m^3), and is linearly related to it using the expression

$$C = Zf$$

Z is a proportionality constant or fugacity capacity with units of $mol/m^3.Pa$ which is specific to the chemical, the phase in which it resides, and temperature. Values of Z for each chemical in each phase can be calculated from appropriate chemical property data and the nature of the phase.

The fugacity (f) or partial pressure (Pa) of a chemical in the vapor phase is related to the concentration (mol/m^3) through the familiar gas law expression

$$C = n/V = P/RT = f/RT = Zf$$

where:

n = number of moles
V = volume (m^3)
R = gas constant (8.314 $Pam^3/mol\ K$)
T = absolute temperature (K)
Z = fugacity capacity, ie. (1/RT) or approximately $4x10^{-4}$ mol/m^3Pa.

If an equilibrium (or equal fugacity) partition coefficient, K_{12}, is known for the chemical between air (1) and another phase (2), such as water solution, then

$$C_1/C_2 = K_{12} = Z_1f/Z_2f = Z_1/Z_2$$

It follows that Z_2 can be calculated as Z_1K_{12}. For air-water equilibrium, the partition coefficient K_{AW} is a form of Henry's Law Constant, ie.

$$K_{AW} = C_A/C_W = H/RT$$

where H is the Henry's Law Constant (Pa m^3/mol), usually expressed as the ratio of chemical vapor pressure P^S (Pa) to solubility C^S (mol/m^3) , ie. P^S/C^S. It follows that for water, Z_W is 1/H or C^S/P^S.

Similarly, for biomass-water partitioning, the partition coefficient, K_{BW} is Z_B/Z_W, thus enabling Z_B to be calculated. A convenient method of estimating K_{BW}, and thus Z_B, is to assume that the biomass is equivalent in composition to a mixture of 20% octanol and 80% water (Blackburn et al., 6), ie.

$$Z_B = 0.2K_{OW}Z_W + 0.8Z_W$$

where K_{OW} is the octanol-water partition coefficient. This is equivalent to a correlation that

$$K_{BW} = Z_B/Z_W = 0.2K_{OW} + 0.8$$

To calculate the Z values of a specific organic chemical, data are thus required for

molecular weight	W (g/mol)
water solubility	S (g/m^3) or C^S (mol/m^3)
vapor pressure	P^S (Pa)
octanol-water partition coefficient	K_{OW}

The Z values are then calculated for

air	as $Z_A = 1/RT$
water	as $Z_W = 1/H = C^S/P^S = S/P^SW$
biomass	as $Z_B = 0.2\ K_{OW}Z_W + 0.8Z_W$

Fugacity, rather than concentration, is used as the descriptor of extent of presence of chemical in each fluid. An advantage of fugacity is that it clearly shows the direction of,

or potential for, diffusive transfer. When the driving force for diffusion is a displacement from equilibrium, it can be expressed as a fugacity difference.

The rates of transport and transformation processes are uniformly expressed in terms of D values or fugacity rate parameters. The rate is then Df mol/h. Three types of D values are used.

For transfer by flow, the rate is conventionally GC mol/h, where G is the flowrate of the phase (m^3/h) and C is concentration mol/m^3. Replacing C by Zf and equating D to GZ gives the rate as Df. This expression is used for flows of water, air, and biomass from vessels.

For reaction or degradation, the rate is conventionally VCk, where V is the phase volume, k is a first order rate constant, and C is concentration. Again, replacing C by Zf and equating D to VZk gives the rate as Df.

The rate of diffusive transfer or vaporization of chemical from the surface of water in vessels to air can be expressed in terms of an overall mass transfer coefficient (K_O) and area (A) product, e.g.

$$\text{Rate} = K_O A(C_W - C_A/K_{AW})$$

where the term in parentheses is the displacement from equilibrium and is thus the driving force for diffusion. Substituting $Z_W f_W$ for C_W, $Z_A f_A$ for C_A, and Z_A/Z_W for K_{AW} gives

$$\text{Rate} = K_O A Z_W (f_W - f_A) = D_O (f_W - f_A)$$

Conventionally, the overall coefficient, K_O, can be expressed as the combination of the water side and air side mass transfer coefficients, K_W and K_A, respectively, ie.

$$1/K_O = 1/K_W + 1/K_A K_{AW}$$

It can be shown that this is equivalent to

$$1/D_O = 1/D_W + 1/D_A$$

where D_W is $K_W A Z_W$ and D_A is $K_A A Z_A$

If estimated values of K_W and K_A and area are available, the values of K_O, D_W, D_A, and D_O can be calculated. In the model K_W is assigned a value of 0.05 m/h and K_A a value of 5 m/h for all chemicals. Chemical or system specific values can be substituted if desired.

For air stripping, two approaches are possible. Values of mass transfer coefficients and areas (or their product) that can be estimated and a D value deduced to give a calculated exit air fugacity or approach to equilibrium. This approach has been used by Roberts et al. (10). Alternatively, and more simply, it can be assumed that the D value is sufficiently large, as a result of sufficiently intimate contacting, that equilibrium (equal fugacity) is reached between the exit air and the water. This latter approach is used here.

Table 1 Steady State Mass Balance Equations

Primary Tank

$$E = f_P(D2 + D3 + DPV + DPB)$$

Aeration Tank

$$D2f_P + D8f_S = f_A(D5 + D6 + DAB)$$

Settling Tank

$$D6f_A = f_S(D7 + D8 + D9 + DSV + DSB)$$

Solution

$$f_P = E/(D2 + D3 + DPV + DPB)$$

$$f_A = D2f_P/[D5 + D6 + DAB - (D8.D6)/(D7 + D8 + D9 + DSV + DSB)]$$

$$f_S = D6f_A/(D7 + D8 + D9 + DSV + DSB)$$

where

f is fugacity (Pa) subscripted P primary: A aeration: S settling

E is influx of chemical (mol/h)

D2 is D value of stream 2 etc., i.e. GZ

DPV and DSV are volatilization D values for primary and settling tanks

DPB, DAB and DSB are biodegradation D values for the three tanks

From a knowledge of the D values, all mass transport and transformation rates can be expressed in terms of the prevailing fugacities; steady state mass balance equations can be written as shown in Table 1, and solved for the fugacities. The various concentrations and rates can be calculated and an entire mass balance assembled for the chemical.

The model can also be modified to calculate the fate of a chemical when the biological waste sludge is returned into the primary settling tank and is wasted, together with the primary sludge.

A computer program has been written to undertake these calculations from the input data.

The output consists of parts which may be printed as requested. Figure 4 gives a complete illustrative output. Part 1 gives the chemical properties, Z values and D values. Part 2 gives specifications of vessels, contents and streams. Part 3 gives the overall chemical mass balance. Part 4 gives a schematic diagram and Part 5 a narrative summary.

PREDICTED FATE OF AN ORGANIC CHEMICAL
IN A WASTEWATER TREATMENT FACILITY

PART 1 : PROPERTIES OF TOLUENE

Molecular weight (g/mol)			92
Aqueous solubility (g/m3)			515
Vapour pressure (Pa)			3800
(atm)			3.750308E-02
(mm Hg)			28.50234
Henry's law constant (Pa.m3/mol)			678.835
Air-water partition coeff (dimensionless)			.273992
Octanol-water partition coefficient (Kow)			389.045
Log Kow			2.59
Biomass to water partition coefficient (d'less)			78.609
Temperature [deg C]			25
Biodeg.rate consts (h^-1),half times in biomass (h) and in 2000 mg/L MLSS (h)			
-Primary tank	.1700297	4.075758	30
-Aeration tank	1.700297	.4075758	3
-Settling tank	1.700297	.4075758	3

Z Values

Z value of chemical in air	4.03621E-04
Z value of chemical in water	1.473112E-03
Z value of chemical in biomass	.1157999

D Values

D value of stream no 1	1.496272
D value of stream no 2	1.478841
D value of stream no 3	1.743146E-02
D value of stream no 5	3.616444
D value of stream no 6	3.168471
D value of stream no 7	1.449187
D value of stream no 8	1.687641
D value of stream no 9	3.164327E-02

Vessel	Primary	Aeration	Settling
Volatilization D value	1.894987E-02	3.616444	5.168148E-02
Biodegradation D value	9.975972E-02	3.937885	.2990629

Figure 4A Illustrative output (Part 1).

```
PART 2 : SPECIFICATION OF VESSELS AND CONTENTS

 Vessel                                Primary        Aeration       Settling
Volume of water m3                     1013.333       8000           2763.636
Volume of biomass m3                   5.066667       20             1.518902
Area m2                                266.6667                      727.2727
Aeration rate m3/h                                    8960
Hydraulic retention time h             1.013333       4.450379       1.537403
Solids retention time h                25.33334       4.450379       .3379843
Volume of water m3                     1013.333       8000           2763.636
Chemical concn (total) mol/m3          1.381165E-04   1.906234E-05   1.496334E-05
Chemical concn (water) mol/m3          9.914718E-05   1.593146E-05   1.434364E-05
Chemical concn (biomass) mol/m3        7.793861E-03   1.252356E-03   1.127539E-03
Fugacity of chemical Pa                6.730458E-02   1.081483E-02   9.736964E-03
Chemical concn (total) g/m3            1.270672E-02   1.753736E-03   1.376627E-03
Amount of chemical g                   12.87614       14.02989       3.804496
Amount of chemical mol                 .139958        .1524988       4.135322E-02
Concentration of VSS g/m3              5000           2500           549.6026

Overall solids retention time (h)                     221.4349

Biodegradation rate  g/h               .6177143       3.918055       .2679007
Total biodegradation rate g/h          4.80367
Total biodegradation rate mol/h        .0522138

Volatilization rate  g/h               .117338        3.598232       .0462963
Total volatilization rate g/h          3.761866
Total volatilization rate mol/h        4.088985E-02

Specification of streams

 # 1 Influent          Water          VSS            Chemical       Air
Flow  m3/h             1000
Flow  g/h                             200000         10
Flow  mol/h                                          .1086957
Concn g/m3                            200            .01
Concn mol/m3                                         1.086957E-04
Fugacity Pa                                          7.264431E-02

 # 2 Prmy effint       Water          VSS            Chemical       Air
Flow  m3/h             997.6
Flow  g/h                             80000          9.157012
Flow  mol/h                                          9.953274E-03
Concn g/m3                            80.19246       9.179041E-03
Concn mol/m3                                         9.977219E-05
Fugacity Pa                                          6.730458E-02

 # 3 Prmy sludge       Water          VSS            Chemical       Air
Flow  m3/h             2.4
Flow  g/h                             120000         .1079359
Flow  mol/h                                          1.173217E-03
Concn g/m3                            50000          .0449733
Concn mol/m3                                         4.888402E-04
Fugacity Pa                                          6.730458E-02
```

Figure 4B Illustrative output continued (Part 2). Specifications of vessels and contents.

# 4 Air inflow	Water	VSS	Chemical	Air
Flow m3/h				8960
Flow g/h			0	
Flow mol/h			0	
Concn g/m3			0	
Concn mol/m3			0	
Fugacity Pa			0	

# 5 Air outflow	Water	VSS	Chemical	Air
Flow m3/h				8960
Flow g/h			3.598232	
Flow mol/h			3.911122E-02	
Concn g/m3			4.015884E-04	
Concn mol/m3			4.365091E-06	
Fugacity Pa			1.081483E-02	

# 6 Aertn efflnt	Water	VSS	Chemical	Air
Flow m3/h	1797.6			
Flow g/h		4494000	3.152515	
Flow mol/h			3.426647E-02	
Concn g/m3		2500	1.753736E-03	
Concn mol/m3			1.906235E-05	
Fugacity Pa			1.081483E-02	

# 7 Final efflnt	Water	VSS	Chemical	Air
Flow m3/h	982.6			
Flow g/h		14739	1.298182	
Flow mol/h			1.411068E-02	
Concn g/m3		15	1.321171E-03	
Concn mol/m3			1.436055E-05	
Fugacity Pa			9.736964E-03	

# 8 Retn sludge	Water	VSS	Chemical	Air
Flow m3/h	800			
Flow g/h		4396821	1.51179	
Flow mol/h			.0164325	
Concn g/m3		5496.026	1.889737E-03	
Concn mol/m3			2.054062E-05	
Fugacity Pa			9.736964E-03	

# 9 Waste sludge	Water	VSS	Chemical	Air
Flow m3/h	15			
Flow g/h		82440.38	2.834606E-02	
Flow mol/h			3.081093E-04	
Concn g/m3		5496.026	1.889737E-03	
Concn mol/m3			2.054062E-05	
Fugacity Pa			9.736964E-03	

Figure 4C Illustrative output continued (Part 2). Specifications of streams.

PART 3 : OVERALL CHEMICAL MASS BALANCE

	g/h	mol/h	percent
Influent	10	.1086957	100.000
Primary sludge	.1079359	1.173217E-03	1.079359
Waste sludge	2.834606E-02	3.081093E-04	.2834606
Primary volatilization	.117338	1.275413E-03	1.17338
Settling volatilization	.0462963	5.032206E-04	.462963
Aeration off gas	3.598232	3.911122E-02	35.98232
Primary biodegradation	.6177143	6.714286E-03	6.177143
Settling biodegradation	.2679007	2.911965E-03	2.679007
Aeration biodegradation	3.918055	4.258755E-02	39.18055
Final water effluent	1.298182	1.411068E-02	12.98182
Total removal	8.701818	9.458497E-02	87.01818
Total biodegradation	4.80367	.0522138	48.0367

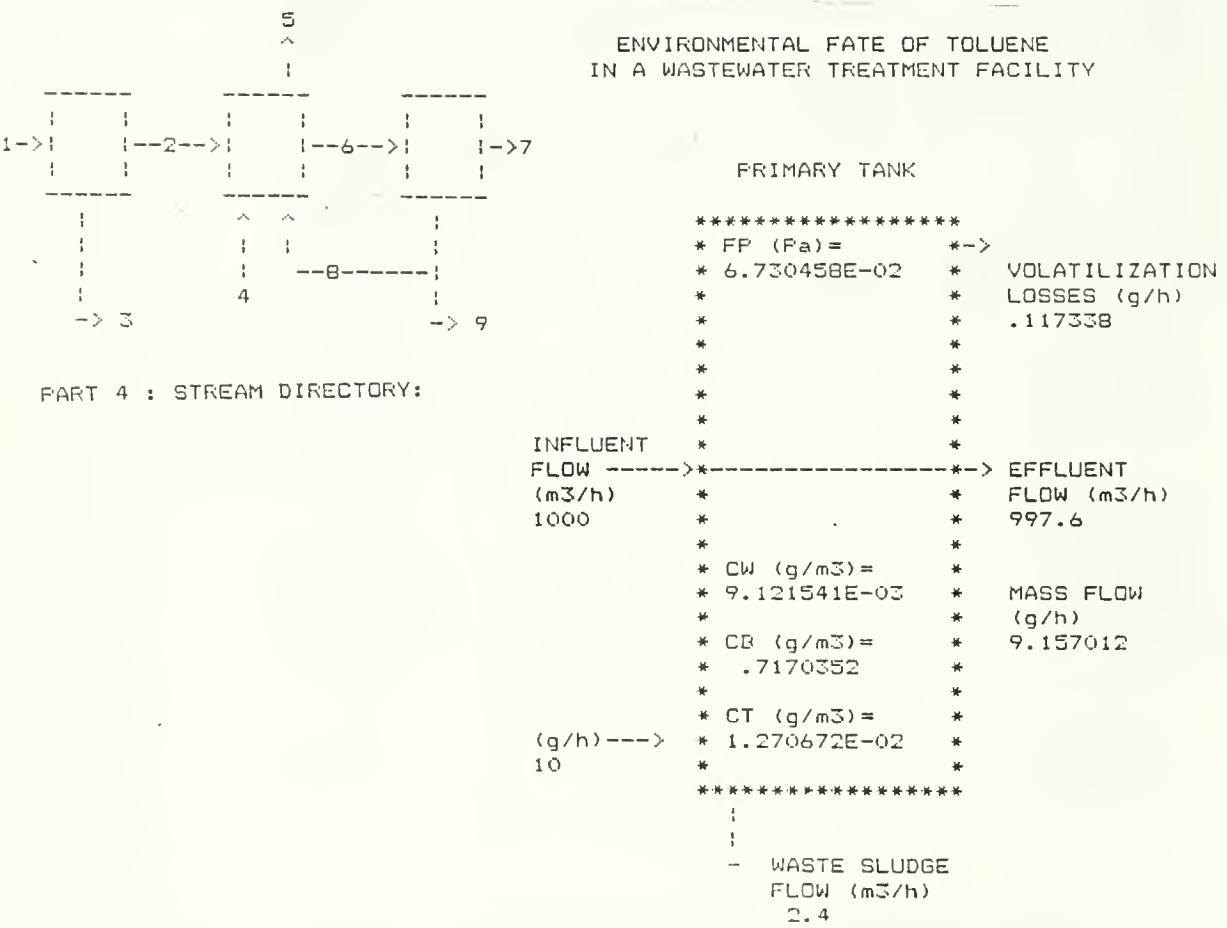

Figure 4D Illustrative output (Part 3 and 4).

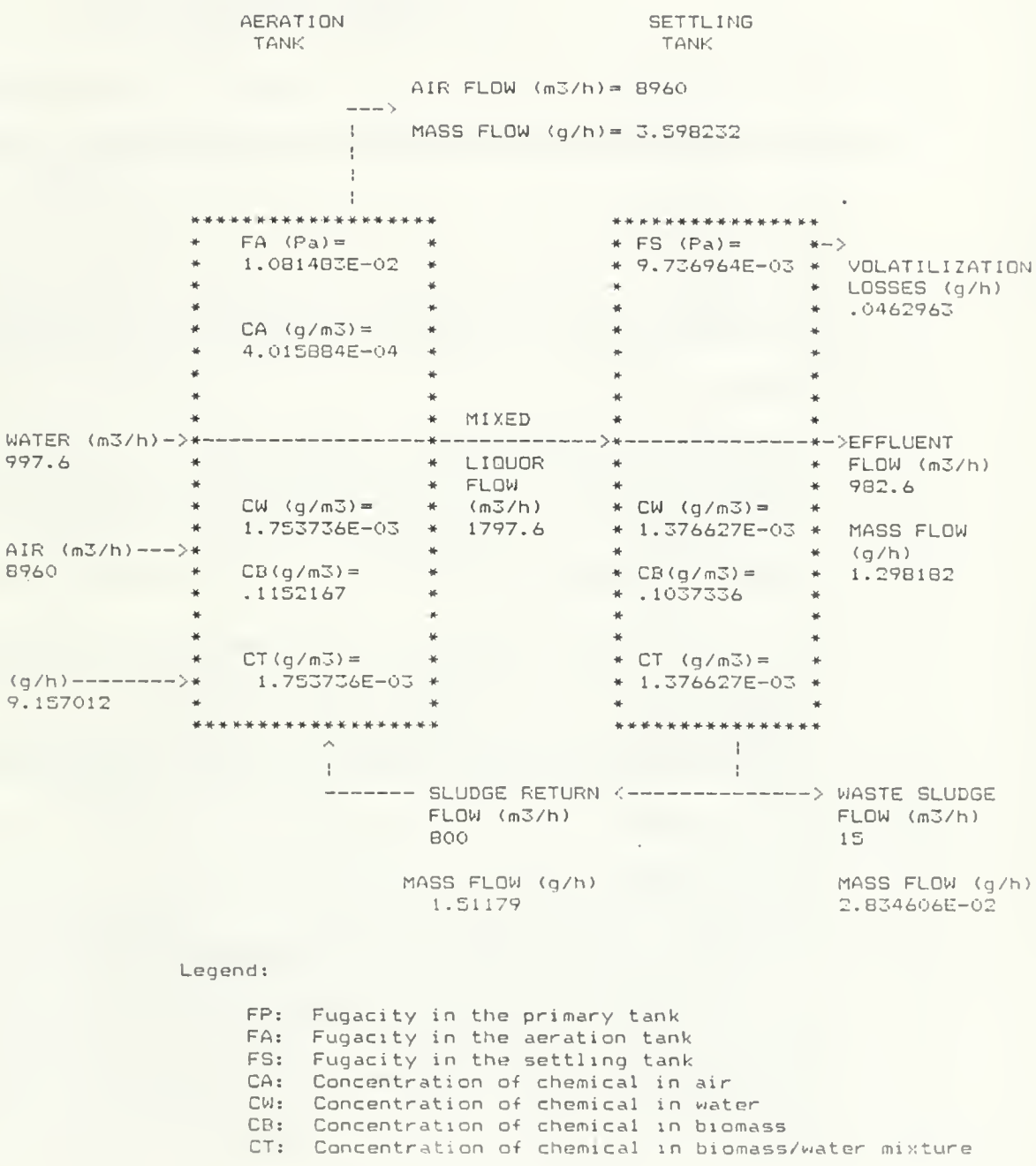

Figure 4E Illustrative output (Part 4 continued).

PART 5 ENVIRONMENTAL FATE OF TOLUENE
IN A WASTEWATER TREATMENT FACILITY
A NARRATIVE SUMMARY

Inflow

The chemical enters the plant at a concentration of 0.01000 g/m3 or mg/L in a total water flow of 1000.0 m3/h ,and thus a flowrate of 10.00 g/h

Primary Settling Tank

During primary treatment, 1.08 percent of the chemical is removed due to sorption to the volatile suspended solids present in the primary tank. It is estimated that 1.17338 percent is volatilized to the atmosphere. Biodegradation accounts for a 6.177143 percent reduction of the chemical. This results in a primary effluent concentration of 0.009179 g/m3 in the water and 0.04497 g/m3 in the sludge.

Aeration Tank

The primary effluent enters the aeration tank at a flowrate of 997.6 m3/h. The air flowrate into the tank is 8960.0 m3/h. Under these conditions, 35.982320 percent of the chemical is removed by stripping and 39.18055 percent is removed by biodegradation. This results in an effluent concentration of 0.00175 g/m3
The concentration of the chemical in the off-gas stream is 0.000402 g/m3.

Secondary Settling Tank

After aeration, the mixed liquor, flowing at 1797.6 m3/h into the secondary tank where settling occurs. This results in the volatilization of 0.46 percent of the chemical and a decrease of 2.679007 percent due to biodegradation. It is estimated that the effluent water concentration is 0.0013 g/m3 and the flowrate is 982.6 m3/h. The underflow is divided into two streams; return sludge and waste sludge to primary which flow at 800.0 m3/h and 15.0 m3/h respectively. The chemical concentration in the sludge is 0.00189 g/m3.

Overall Summary

The chemical enters the plant at a flow rate of 10.000000 g/h.
Of this 37.61867 percent or 3.7619 g/h of the chemical will transfer to the atmosphere, of which35.98232 percent or 3.5982 g/h is stripped.
A total of 48.03670 percent or 4.8037 g/h is biodegraded.
The primary sludge stream removes 1.07936 percent or 0.1079 g/h, and the waste sludge stream removes 0.28346 percent or 0.0283 g/h.
The concentration of the chemical in the air off-gas is 0.00040 g/m3.
The primary sludge concentration is 0.0450 g/m3; and the waste sludge concentration is 0.0019 g/m3.
The secondary effluent concentration is 0.001321 g/m3. The net result is that the sewage treatment plant is 87.01818 percent effective for the removal of this chemical

Figure 4F Illustrative output (Part 5). Narrative summary.

Illustration

Figure 4 gives the model output and properties for toluene. Toluene was selected to give a significant amount of chemical being removed by each process. The toluene mass balance is also illustrated in Figure 1C.

The chemical is present at 0.01 g/m^3 in the influent of 1000 m^3/h giving an inflow of 10 g/h. About 29% of the chemical is sorbed to the biomass in the contents of the primary clarifier since K_{BW} is about 79 and the biomass volume fraction in the tank is about 1/200. The water has a shorter retention time (1h) than the solids (25h) thus most of the chemical leaves with the effluent water (9.16 g/h), with 0.11 g/h leaving with the sludge, 0.12 g/h volatilizing and 0.62 g/h biodegrading.

In the aeration tank there is 20 m^3 of biomass and 8000 m^3 water ie a MLSS of 2500 g/m^3. The chemical partitions about 84% into the water and 16% in the biomass. The half time of the biodegradation process in the biomass is 0.4 hours while in the MLSS it is about 3 hours because of the partial partitioning into the biomass. The retention time is 4.4h, thus about one third of the chemical (3.92 g/h) is degraded. The aeration tank off gas removes 3.6 g/h, the air volumetric flow being about equal to the water volumetric flow per hour and the air/water partition coefficient is fairly high (0.27). The chemical concentration in the air is thus about 0.0004 g/m^3 or quarter the dissolved chemical concentration in the water of 0.0017 g/m^3. Since 1.51 g/h return to the aeration tank with the recycled sludge (giving a total inflow of about 10.67 g/h) the effluent contains the balance or 3.15 g/h.

In the final settling tank the chemical is subject to only slow volatilization (0.05 g/h) and biodegradation (0.27 g/h), there being about an equal split between the water effluent (1.30 g/h) and the sludge (1.54 g/h). The sludge is mainly recycled with 0.03 g/h of chemical leaving in the waste sludge and 1.51 g/h being recycled. The final effluent contains 1.3 g/h of chemical in about 55% of the water entering the settling vessel.

Overall, of the 10.0 g/h inflow, 4.80 is biodegraded, 3.76 volatilizes and 0.14 is sorbed to sludges (totalling 8.7) g/h, and 1.3 g/h leaves in the final effluent. The overall efficiency of removal is thus 87%, but only 48% is chemically destroyed.

In terms of fugacity, the initial value of .0726 Pa falls slightly to 0.0673 Pa in the primary tank because of slight volatilization and biodegradation. Since the process is simply equilibrium separation there is no substantial fugacity change. In the aeration stage the fugacity drops to 0.0108 Pa (i.e. by a factor of 6.2) as a result of reaction and volatilization. There is another slight drop to 0.0097 Pa in the settling tank. It is this factor of 6.2 which controls the overall removal efficiency of 87%, i.e. approximately 1/6.2 or 16% is untreated. Overall, the STP has achieved a fugacity reduction by a factor of 7.5.

Essentially, the plant removes about 60% of the sorbed chemical in the primary vessel, at the influent fugacity. It then reduces the fugacity of the chemical in the water by a factor such as 6.2 by biodegradation and volatilization, then separates most of the remaining sorbed chemical at this lower fugacity. For very highly sorbed persistent chemicals, the fugacity reduction factor is of little importance, the principal function of the plant being the

physical separation of sludge. For poorly sorbed chemicals the factor is critical and controlling. Since the waste sludge is always at a lower fugacity than the primary tank content it is always thermodynamically disadvantageous to recycle this sludge to the primary tank since it involves mixing streams of unequal concentration.

A SIMPLIFIED MODEL

This analysis suggests that the plant could be modelled in a very simple approximate manner using D values for certain key streams namely D2, D3, D5, D7 and D9. The chemical inflow will split in the primary tank approximately as D2/(D2+D3) to the aeration tank and D3/(D2+D3) to the sludge. The flow to the aeration tank will eventually split approximately in the proportions DB (biodegradation), DV (volatilization), D7 (effluent) and D9 (waste sludge). The amounts removed by various processes will thus be:

Biodegradation	DB.D2/[(D2+D3)(DB+DV+D7+D9)]
Volatilization	DV.D2/[(D2+D3)(DB+DV+D7+D9)]
Effluent	D7 D2/[(D2+D3)(DB+DV+D7+D9)]
Sludges	D3/(D2+D3) + D9.D2/(D2+D3)(DB+DV+D7+D9)

These fractions total to unity.

These D values can be estimated from the flows of waste biomass and air, the rate constant and the corresponding volume of biomass. For simplicity it may be preferable to ignore biodegradation and volatilization in the primary and settling tanks.

This simple calculation is illustrated below. For toluene ZA is 0.00040, ZW is 0.00147 and ZB is 0.116.

D2 is approximately

water 1000 m^3/h x ZW or 1.47

biomass 0.08 m^3/h x ZB or 0.009 Total 1.48

D3 is approximately

water 2.4 m^3/h x ZW or 0.003

biomass 0.12 m^3/h x ZB or 0.014 Total 0.017

DV is approximately

8960 m^3/h x ZA or 3.58 Total 3.58

D7 is approximately

water 983 x ZW or 1.44

biomass .015 x ZB or 0.0017 Total 1.44

D9 water 15 x ZW or 0.022

biomass 0.082 x ZB or 0.0095 Total 0.032

DB 20 m^3 x 1.70 h^{-1} x ZB or 3.94 Total 3.94

Note that the rate constant of 1.7 h^{-1} is deduced from the half life of 3 hours at a MLSS of 2000. At 2000 g/m^3 the fraction dissolved is

$$1/(1 + 2000 \times K_{BW}/10^6) = 0.864$$

where K_{BW} is the biomass water partition coefficient or ZB/ZW or 79. The fraction sorbed is thus 0.136. Thus to achieve an overall rate constant of 0.693/3 or 0.231 h^{-1} requires a rate constant of 0.231/0.136 or 1.70 h^{-1} in the biomass phase.

The group $(D2+D3)(DB+DV+D7+D9) = 13.46$

The proportions are thus

Biodegradation	43%	
Volatilization	39%	
Waste Effluent	16%	
Sludges	2%	Total 100%

This is in fair agreement with the amounts calculated by the more complex model.Given the errors in analyses, the variations and uncertainty in conditions, this simple approach may be sufficiently accurate for may practical purposes. It has the advantage that the relative importance of the key processes becomes readily apparent.

Comparison with Full Scale STP Performance

Monteith (5) has reported an extensive compilation of trace organic chemical removal efficiency in STPs. Table 2 is a summary of selected data from that report, specifically from Tables 77, 80, 84 and 85 which give data for STPs in Toronto, Ohio, Wisconsin, the EPA 40 POTW study and the EPA 30 day study. More weight was assigned to the last two studies. It is striking that there is considerable variability in the efficiencies, probably as a result of (i) design and operating differences, (ii) analytical errors and (iii) fluctuations in concentration giving rise to a mismatch of influent and effluent as well as variation in

Table 2 Removal efficiencies reported by Monteith (5) and as estimated by the model.

Chemical	Overall Removal Efficiency			Percent Contributions of Removal Processes				Model Estimates				
								Removal Efficiency	Percents			
	Low	Med	High	Volat	Biodeg	Sludge	Efflt		Volat	Biodeg	Sludge	Efflt
111 trichloroethane	71	85	94	74	10	1	15	92	85	7	<1	8
112 trichloroethene	82	85	97	64	15	6	15	82	68	14	<1	18
toluene	70	85	95	20	55	15	10	87	38	48	1	13
14 dichlorobenzene	57	70	80	40	10	20	30	65	25	33	7	35
naphthalene	65	85	95	15	55	15	15	73	6	59	8	27
anthracene	60	80	90	0	30	50	20	80	<1	37	42	20
pyrene	70	85	90	0	0	85	15	87	<1	30	57	13
dibutylphthalate	60	65	87	0	45	20	35	78	<1	30	48	22
2 ethyl hexyl phthalate	40	50	80	0	25	25	50	97	<1	27	70	3
dioctylphthalate	20	85	98	0	80	5	15	96	<1	20	75	4
phenol	90	98	99	0	98	0	2	97	<1	97	<1	3
pentachlorophenol	20	75	85	0	75	10	15	99	<1	65	34	1
2,4D	40	60	80	0	60	0	40	71	<1	68	2	29

Table 3 Physical chemical properties of the test chemicals at 25°, most data being from references 17 and 18, with estimated biodegradation half lives under aeration conditions at MLSS of 2000 mg/L.

Chemical	Molec. Mass g/mol	Water Solubility g/m^3	Vapor Pressure Pa	K_{ow}	Biodeg. Half life (hours)
111 trichloroethane	133.4	700	13200	2.3	20
112 trichloroethene	131.4	1100	8000	2.3	15
toluene	92	515	3800	2.6	3
14 dichlorobenzene	147.0	80	90	3.4	20
naphthalene	128.1	33	11	3.5	10
anthracene	178.2	.046	$1.44x10^{-3}$	4.5	60
pyrene	202.2	0.135	$8.9x10^{-4}$	4.9	100
dibutylphthalate	278.3	10	.01	4.6	100
2 ethyl hexyl phthalate	390.5	0.04	$3x10^{-4}$ (?)	6.0 (?)	100
dioctylphthalate	390.5	0.04	$3x10^{-4}$	6.0 (?)	200
phenol	94.1	90000	57	1.46	0.5
pentachlorophenol	266.3	14	$1.5x10^{-2}$	5.0	10
2,4D	221.0	890	$6x10^{-5}$	2.8	5

removal efficiency. These efficiency data were treated to remove some outliers, then the upper and lower quartiles and a mean were estimated. These are reported in Table 2. For example, it is believed that toluene will normally be removed with an efficiency between 70 and 95%, with 85% being an average efficiency, a figure close to the EPA values of 86 and 83%. It is emphasised that there is a strong element of judgement in this process.

Monteith (5) also compiled (in his Table 97) estimates of the relative importance of removal mechanisms from a variety of sources. Averages were taken and are given in Table 2, some obvious outliers being removed and consistency being obtained with the overall removal efficiency data. These data are believed to be the best available for testing the model for its ability to reproduce the fate of chemicals in a typical Ontario STP. No attempt has been made to run the model for specific designs and operating conditions, because this information is generally not available.

The model was then run for these chemicals using the physical chemical properties in Table 3 yielding the results given in Table 2. A key parameter which must be selected is the biodegradation half life, values being given in Table 3. This is the only "fitted" parameter and is not, of course, an inherent measurable physical-chemical property such as solubility. When there is appreciable volatilization and removal in sludge, it is necessary to use a model such as this to "back out" a biodegradation half life from the reported STP performance data. In all cases the most biodegradation takes place in the aeration and settling vessels, it being assumed that the most biodegradation half lives are a factor of 3 to 5 longer in the primary vessel.

The dominance of volatilization for the chlorinated ethane and ethene chemicals is well reproduced. The aromatics are well simulated with volatilization becoming less important as vapour pressure drops. 24D is also well predicted. In all these cases the estimated removal efficiency lies in range reported.

The phthalate esters are less well simulated. The model correctly predicts negligible volatilization, but it predicts higher partitioning to sludge than is apparently observed. It appears that the "effective" K_{ow} is lower than the true value. A similar effect is apparent with pentachlorophenol in which volatilization and biodegradation are well predicted, but there is apparently less sorption. Reducing log K_{ow} from 5 to 4 to account for ionization and thus reduced partitioning gives an improved simulation with less sorption and a lower removal efficiency of 86%.

Phenol is readily degraded as expected.

It is thus concluded that the model can be used, with appropriate caution, to fit other data and estimate the fate of other similar chemicals, provided that biodegradation rate estimates are available. Although not tested here, it is believed that the model could be used to explore the effect of variations in operating conditions such as aeration or recycle rates and sludge retention times.

There is an obvious need for reliable full scale plant mass balance data from which biodegradation and sorption information can be obtained. It is probable that the expression for sorption to biomass can be improved, especially for ionizing chemicals.

CONCLUSIONS

A novel interactive fugacity-based model has been developed to describe the fate of organic chemicals in sewage treatment plants. It describes the partitioning, biodegradation and volatilization or stripping behavior of the chemical and compiles an overall mass balance. The validity of the model has been assessed by comparing the model's estimates of fate of 13 chemicals using only a single fitted biodegradation half life parameter. It is believed that the model will be useful for estimating the likely fate of various chemicals and for exploring the effect of various operating conditions.

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